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NAVIER-STOKES EQUATIONS

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During this period we initiated work on modeled PDF, i.e., PDF's that are governed by an evolution equation. An abstract¹ was submitted to the AIAA/SAM/ASME/ASEE 30th Joint Propulsion Conference and Exhibit. A copy of the abstract is enclosed.

1. Baurle, R. A., Hsu, A. T., and Hassan, H. A., "Comparison of Assumed and Evolution PDF's in Supersonic Turbulent Combustion Calculations", Abstract submitted to the 30th Joint Propulsion Conference and Exhibit.

Comparison of Assumed and Evolution PDF's in Supersonic Turbulent Combustion Calculations

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The objective of this study is to compare the use of assumed pdf (probability density function) approaches for modeling supersonic turbulent reacting flowfields with the more elaborate approach where the pdf evolution equation is solved. Assumed pdf approaches for averaging the chemical source terms require modest increases in CPU time typically of the order of 20 % above treating the source terms as "laminar". However, it is difficult to assume a form for these pdf's a priori that correctly mimics the behavior of the actual pdf governing the flow. Solving the evolution equation for the pdf is a theoretically sound approach, but because of the large dimensionality of this function, its solution requires a Monte Carlo method which is computationally expensive and slow to converge. Preliminary results show both pdf approaches to yield similar solutions for the mean flow variables.

Introduction

In order to obtain accurate predictions for turbulent reacting flowfields, the effect of turbulence on the chemical source terms must be addressed. These source terms are highly nonlinear functions of both temperature and composition and as a result employing typical time averaging is difficult. An attractive alternative for obtaining these averages is to utilize pdf models which can be used to obtain averages for functions of any form. These pdf approaches consist of two types. The first being the assumed pdf approach where the pdf

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is completely defined knowing only the first couple of moments, and the second approach where an evolution equation is solved for the pdf.

Many assumed forms for pdf's have been used for obtaining averages for the chemical source terms in supersonic reacting flows. All of these forms have either neglected the effects of composition fluctuations, or assumed statistical independence between the temperature and the composition. Frankel et al.¹ examined the effects of temperature fluctuations on the chemical source terms using both Gaussian and Beta forms for the pdf. Both assumed forms yielded similar results and showed modest improvements over treating these source terms in a laminar fashion when compared to experiment. Later Narayan and Girimaji² combined a moment method to account for temperature fluctuations with a multi-variate Beta distribution developed by Girimaji³ to account for composition fluctuations. Their results showed the effect of the multi-variate Beta distribution to be minimal on the mean flow variables. This same behavior was seen later by Baurle et al.⁴

The use of evolution pdf methods for low speed turbulent reacting flows have been examined extensively.^{5, 6, 7} However, until recently⁸, the extension of these methods to high speed flows has been practically non-existent due to difficulties arising from shocks and strong dilatation terms. Hsu et al.⁸ solved the evolution equation for the joint pdf of specific enthalpy and mass fractions in conjunction with a CFD flow solver for the Navier-Stokes equations. Significant improvements over calculations without the pdf were noted when compared to experimental data for high speed reacting flows.

The Assumed Joint PDF Approach

For the assumed pdf approach, the species continuity equations are solved in conjunction with the Navier-Stokes equations. To obtain an average of the chemical source terms ($\dot{\omega}_k$) that appear in the species equations,

$$\dot{\omega}_k = W_k \sum_{l=1}^{nr} (\nu''_{kl} - \nu'_{kl}) \left[k_{f_l} \prod_{m=1}^{ns} \left(\frac{\rho_m}{W_m} \right)^{\nu'_{ml}} - k_{b_l} \prod_{m=1}^{ns} \left(\frac{\rho_m}{W_m} \right)^{\nu''_{ml}} \right] \quad (1)$$

a joint pdf of temperature and composition is needed. In this work, the joint pdf was chosen as

$$\mathcal{P}(T, Y_k) = \mathcal{P}_1(T) \mathcal{P}_2(Y_k) \quad (2)$$

Here, the pdf of temperature ($\mathcal{P}_1(T)$) was chosen as a Gaussian distribution

$$\mathcal{P}_1(T) = \frac{1}{\sqrt{2\pi\widetilde{T''^2}}} \exp \left[-\frac{(T - \widetilde{T})^2}{2\widetilde{T''^2}} \right] \quad (3)$$

and the pdf of the mass fractions ($\mathcal{P}_2(Y_k)$) was chosen as the multi-variate Beta distribution developed by Girimaji³

$$\mathcal{P}_2(Y_k) = \frac{\Gamma(\sum_{k=1}^{ns} \beta_k)}{\prod_{k=1}^{ns} \Gamma(\beta_k)} \left[\delta \left(1 - \sum_{k=1}^{ns} Y_k \right) \prod_{k=1}^{ns} Y_k^{\beta_k - 1} \right] \quad (4)$$

It can be shown that

$$\beta_k = \tilde{Y}_k \left(\frac{1-S}{\sigma_Y} - 1 \right) \quad (5)$$

where

$$S = \sum_{k=1}^{ns} (\tilde{Y}_k)^2, \quad \sigma_Y = \sum_{k=1}^{ns} \widetilde{Y_k''^2} \quad (6)$$

To use this approach the solution of two extra transport equations are required. One for the enthalpy (or temperature) variance and one for the species mass fraction variance sum (σ_Y).

The Evolution Joint PDF Approach

For the evolution pdf approach, the species continuity equations are replaced by the pdf evolution equation. The simulation of this equation yields the mean mass fractions which is all that is required by the Reynold's averaged Navier-Stokes equations. The single point joint pdf evolution equation is derived from the specific enthalpy and species continuity equations. If the dissipation due to viscosity is neglected, this equation can be written as

$$\frac{\partial(\bar{\rho}\tilde{\mathcal{P}})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\tilde{\mathcal{P}})}{\partial x_j} + \frac{\partial(\dot{\omega}_k\tilde{\mathcal{P}})}{\partial \psi_k} = -\frac{\partial(\bar{\rho}\langle u_j'' | \psi_k, \theta \rangle \tilde{\mathcal{P}})}{\partial x_j} - \frac{\partial(\langle \frac{Dp}{Dt} | \psi_k, \theta \rangle \tilde{\mathcal{P}})}{\partial \theta} - M(\psi_k, \theta; x, t) \quad (7)$$

where $M(\psi_k, \theta; x, t)$ represents the effect of molecular mixing, and (ψ_k, θ) are the sample space variables corresponding to the random variables (Y_k, h) . The terms on the right hand side of the above equation require modeling which is discussed in references 7, 8, and 9.

Due to the large dimensionality of the joint pdf, solving this equation with a finite difference approach is not practical since the computational cost can be shown to rise exponentially with the dimensionality of the pdf. The computational cost of a Monte Carlo simulation of the above expression can be shown to rise linearly with the dimensionality of the pdf.¹⁰ Thus, the above equation is simulated using a fractional step Monte Carlo scheme as described in reference 10.

Results and Discussion

The cases considered involved the parallel injection of hydrogen into a supersonic stream of air as shown by the schematic in Figure 1, and results are compared with the experimental data of Beach et al.¹¹ Table 1 gives a summary of the burner exit conditions. Measurements were taken at axial stations of 8.26, 15.5, 21.7, and 27.9 inner diameters downstream of the burner. All computations were carried out using a 61 X 71 grid on a domain of 30 X 2 inner diameters.

The CFD solver employs a cell centered finite volume approach stepped in time using a 4 stage Runge-Kutta scheme. To alleviate the stiffness caused by the different time scales

between the fluid motion and the chemistry, the chemical source terms are treated in a point implicit manner.

For the assumed pdf approach, the 7 step kinetic model by Jachimowski¹² was employed as given in Table 2. Figure 2 compares the calculated mean mass fraction profiles with the experimental data at all 4 axial stations where measurements were taken. As can be seen, fair agreement with experiment is noted at each station. The total cpu time to reach the steady state (5000 iterations) was approximately 860 seconds on a Cray C90.

For the evolution pdf approach, a simpler 2 step kinetic model by Rogers and Chinitz¹³ was employed as given in Table 3. Once again good agreement with experiment is noted, in fact the results are very close to that predicted by the assumed pdf approach where a more elaborate chemistry model was used. One noticeable difference is the location of the peak in the H_2O profile comparisons. It is shifted down somewhat more than in the assumed pdf solution which is consistent with the experimental measurements. The total cpu time to reach the steady state (6000 iterations) was approximately 2640 seconds on a Cray C90.

The final paper will implement a general chemistry model into the pdf Monte Carlo solver so a more meaningful comparison between computational costs and accuracy can be made. Also, more detailed comparisons with the above experiment and comparisons with a more recent experiment conducted by Cheng et al.¹⁴ will be presented.

Acknowledgements

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References

- [1] Frankel, S. H., Drummond, J. P., and Hassan, H. A. "A Hybrid Reynolds Averaged/Pdf Closure Model for Supersonic Turbulent Combustion". AIAA Paper 90-1573, June 1990.
- [2] Narayan, J. R., and Girimaji, S. S. "Turbulent Reacting Flow Computations Including Turbulence-Chemistry Interactions". AIAA Paper 92-0342, Jan. 1992.
- [3] Girimaji, S. S. "A Simple Recipe for Modeling Reaction-Rates in Flows with Turbulent Combustion". AIAA Paper 91-1792, June 1991.
- [4] Baurle, R. A., Alexopoulos, G. A., Hassan, H. A., and Drummond, J. P. "An Assumed Joint-Beta Pdf Approach for Supersonic Turbulent Combustion". AIAA Paper 92-3844, July 1992.
- [5] Pope, S. B. "Pdf Methods for Turbulent Reactive Flows". *Prog. Energy Combustion Science*, Vol. 11:119-192, 1985.
- [6] Kollman, W. "The Pdf Approach to Turbulent Flow". *Theoretical Computational Fluid Dynamics*, Vol. 1:249-285, 1990.

- [7] Hsu, A. T. "A Study of Hydrogen Diffusion Flames Using Pdf Turbulence Model". AIAA Paper 91-1780, June 1991.
- [8] Hsu, A. T., Tsai, Y. L. P., and Raju, M. S. "A Pdf Approach for Compressible Turbulent Reacting Flows". AIAA Paper 93-0087, Jan. 1993.
- [9] Hsu, A. T., and Chen, J. Y. "A Continuous Mixing Model for Pdf Simulations and its Applications to Combusting Shear Flows". In *8th Symposium on Turbulent Shear Flows*, Munich, Sept. 1991.
- [10] Pope, S. B. "A Monte Carlo Method for the Pdf Equations of Turbulent Reactive Flow". *Combustion Science and Technology*, vol. 25:159-174, 1980.
- [11] Evans, J. S., Schexnayder, C. J., and Beach, H. L. "Application of a Two Dimensional Parabolic Computer Program to Prediction of Turbulent Reacting Flows". NASA Technical Paper 1169, March 1978.
- [12] Jachimowski, C. J. "An Analytic Study of the Hydrogen-Air Reaction Mechanism with Application to Scramjet Combustion". NASA Technical Paper 2791, Feb. 1988.
- [13] Rogers, R. C., and Chinitz, W. "Using a Global Hydroden-Air Combustion Model in Turbulent Reacting Flow Calculations". *AIAA Journal*, Vol. 21:No. 4, April 1983.
- [14] Cheng, T. S., Wehrmeyer, J. A., Pitz, R. W., Jarrett, O. Jr., and Northam, G. B. "Finite-Rate Chemistry Effects in a Mach 2 Reacting Flow". AIAA Paper 91-2320, June 1991.

Tables

Table 1: Burner Exit Conditions

Exit Conditions	Inner Jet	Outer Jet
Mach Number	2.0	1.9
Temperature [$^{\circ}K$]	251.0	1495.0
Pressure [MPa]	0.1	0.1
Mass Fraction		
Y_{H_2}	1.0	0.0
Y_{O_2}	0.0	0.241
Y_{N_2}	0.0	0.478
Y_{H_2O}	0.0	0.281
all others	0.0	0.0

Inner Jet Diameter = 0.006525 m

Lip Thickness = 0.0015 m

Outer Jet Diameter = 0.0653 m

Table 2: Abridged Jachimowski Chemistry Model

Reaction	A	b	T_a
$H_2 + O_2 \rightleftharpoons OH + OH$	1.70E+13	0.0	24157.0
$H + O_2 \rightleftharpoons OH + O$	1.20E+17	-0.91	8310.5
$OH + H_2 \rightleftharpoons H_2O + H$	2.20E+13	0.0	2591.8
$O + H_2 \rightleftharpoons OH + H$	5.06E+04	2.67	3165.6
$OH + OH \rightleftharpoons H_2O + O$	6.30E+12	0.0	548.6
$H + OH + M \rightleftharpoons H_2O + M$	2.21E+22	-2.0	0.0
$H + H + M \rightleftharpoons H_2 + M$	7.30E+17	-1.0	0.0

Units of A are a multiple of $\frac{cm^3}{mole \cdot sec}$

Table 3: Rogers and Chinitz Chemistry Model

Reaction	A	b	T_a
$H_2 + O_2 \rightleftharpoons 2OH$	A_1	-10.0	2448.0
$H_2 + 2OH \rightleftharpoons 2H_2O$	A_2	-13.0	21389.0

Units of A are a multiple of $\frac{cm^3}{mole \cdot sec}$

$$A_1 = \left(\frac{31.433}{\phi} + 8.917\phi - 28.95 \right) 10^{47}$$

$$A_2 = \left(\frac{1.333}{\phi} - 0.833\phi + 2.0 \right) 10^{64}$$

Figures

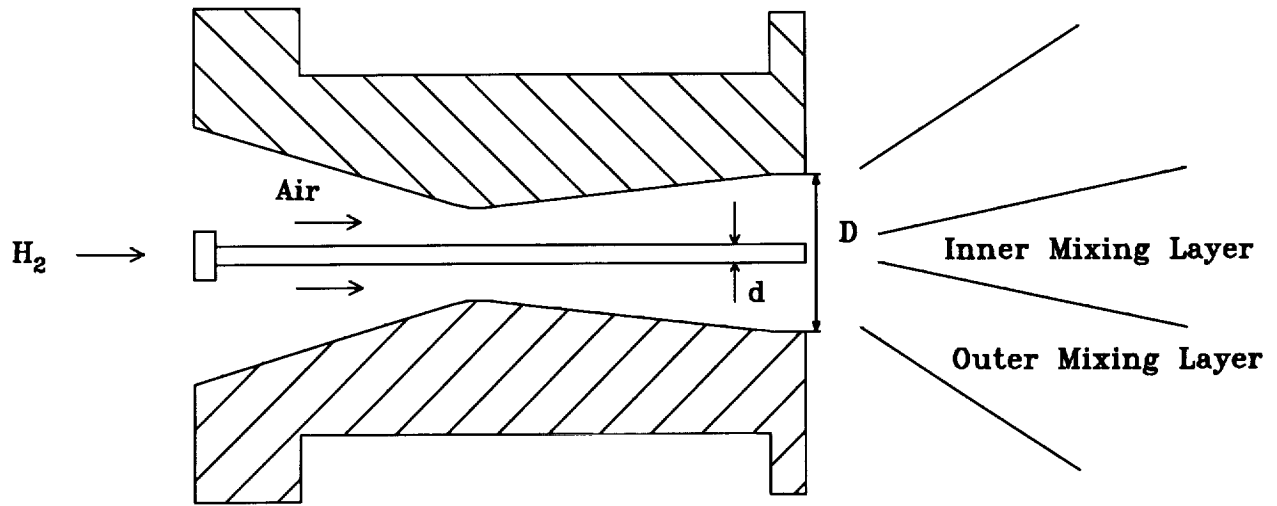


Figure 1. Schematic of Test Apparatus

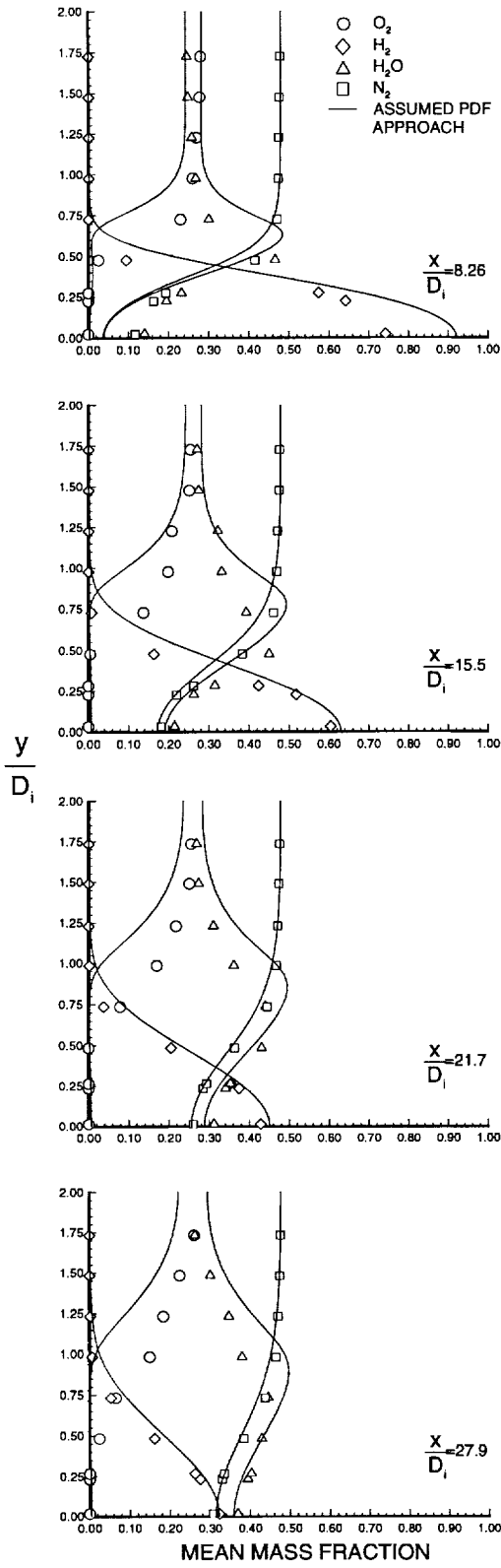


Figure 2. Assumed PDF Comparisons of Mass Fractions with Experiment

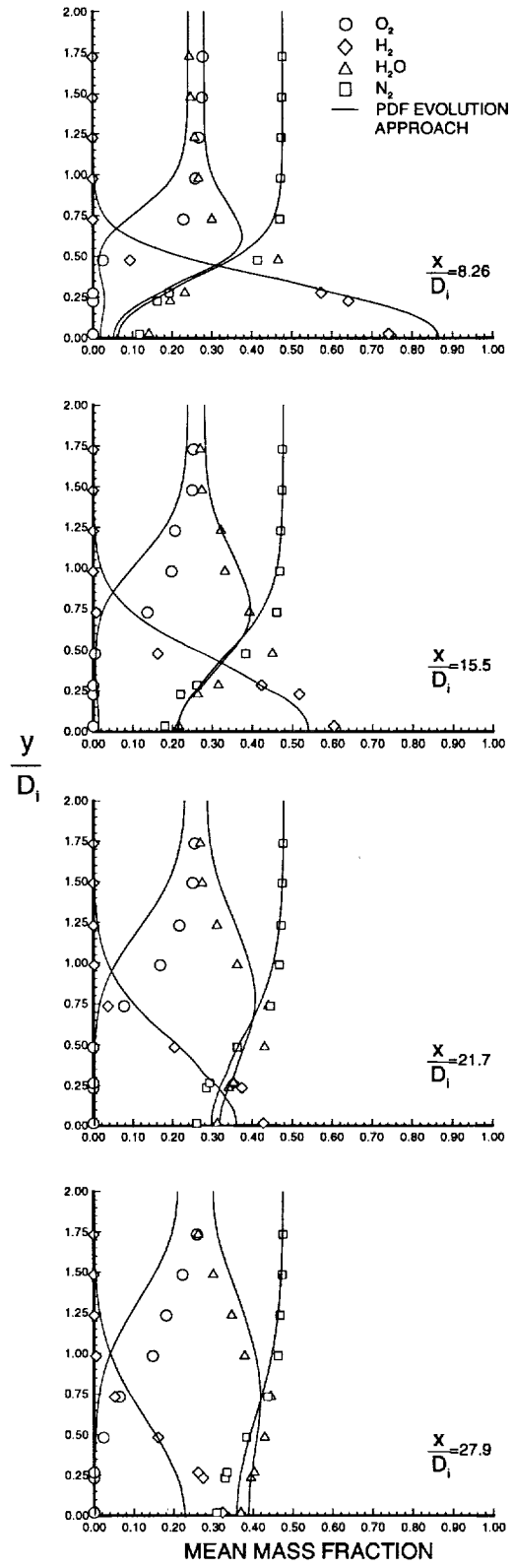


Figure 3. PDF Evolution Comparisons of Mass Fractions with Experiment